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OFFICE OF NAVAL RESEARCH

Contract No. N-00014-86-C-0808

Technical Report No. 4

# ON THE ITERATIVE BOUNDARY ELEMENT METHOD

by
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Submitted to
BETECH90, July 10-12, 1990, University of Delaware

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Subcontract through
The Eveready Battery Company
Westlake, Ohio 44145

15 March 1990

UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

# REPORT DOCUMENTATION PAGE

| | |
|---|---|
| 1a REPORT SECURITY CLASSIFICATION | 1b RESTRICTIVE MARKINGS |
| 2a SECURITY CLASSIFICATION AUTHORITY | 3 DISTRIBUTION AVAILABILITY OF REPORT<br>Approved for public release: distribution unlimited |
| 2b DECLASSIFICATION / DOWNGRADING SCHEDULE | |
| 4 PERFORMING ORGANIZATION REPORT NUMBER(S)<br>Technical Report No. 5 | 5 MONITORING ORGANIZATION REPORT NUMBER(S) |
| 6a NAME OF PERFORMING ORGANIZATION<br>Chemistry Dept. and Case Center for Electrochemical Sciences<br>6b OFFICE SYMBOL (If applicable) | 7a NAME OF MONITORING ORGANIZATION<br>Office of Naval Research<br>Chemistry Code 472 |
| 6c ADDRESS (City, State, and ZIP Code)<br>Case Western Reserve University<br>Cleveland, OH 44106-2699 | 7b ADDRESS (City, State, and ZIP Code)<br>Chemistry Program<br>800 N. Quincy Street<br>Arlington, VA 22217 |
| 8a NAME OF FUNDING / SPONSORING ORGANIZATION<br>Office of Naval Research<br>8b OFFICE SYMBOL (If applicable) | 9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER<br>Contract No. N-00014-86-C- |
| 8c ADDRESS (City, State, and ZIP Code) | 10 SOURCE OF FUNDING NUMBERS<br>PROGRAM ELEMENT NO / PROJECT NO / TASK NO / WORK UNIT ACCESSION NO |

11 TITLE (Include Security Classification)

A Generic I-Biem for Electrochemical Problems

12 PERSONAL AUTHOR(S)
B. D. Cahan and O. Lafe

| 13a TYPE OF REPORT | 13b TIME COVERED FROM ____ TO ____ | 14 DATE OF REPORT (Year, Month, Day) | 15 PAGE COUNT |
|---|---|---|---|
| Interim Technical | | | 10 |

16 SUPPLEMENTARY NOTATION

To be submitted to the Journal of the Electrochemical Society

| 17 COSATI CODES | | | 18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number) |
|---|---|---|---|
| FIELD | GROUP | SUB-GROUP | |
| | | | |
| | | | |

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

A generic computer code based on the iterative boundary integral equation method (I-BIEM) is developed for simulating a variety of electrochemical problems. In this work we have extended the reach of the method by developing a generalized program capable of solving a wide range of electrodeposition problems. The new code accomodates quite easily multi-variable problems including those with curved boundaries, and non-linear boundary conditions. Such problems include anomalous codeposition of alloys, incorporating the effects of convective and diffusive mass transport; time variant effects such as would be observed in extended growth calculations and pulse plating; microstructural modeling with reference to nonisotropic boundary conditions and crystallographic effects. Some interesting results of real-life simulations are presented.

| 20 DISTRIBUTION / AVAILABILITY OF ABSTRACT | 21 ABSTRACT SECURITY CLASSIFICATION |
|---|---|
| ☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS | |
| 22a NAME OF RESPONSIBLE INDIVIDUAL<br>Dr. Robert Nowak | 22b TELEPHONE (Include Area Code)<br>(202) 696-5075 |
| | 22c OFFICE SYMBOL |

DD FORM 1473, 84 MAR 83 APR edition may be used until exhausted
All other editions are obsolete

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

# On the Iterative Boundary Element Method

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## ABSTRACT

A generalized iterative scheme is developed for the solution of a large class of boundary integral equations. The code is an excellent method for solving problems with huge coefficient matrices. The scheme avoids the use of large computer storage spaces and a direct inversion of the matrices is also not required. The result is a considerable improvement over existing boundary element schemes in terms of computer running time and accuracy especially for problems with complex shapes and non-linear boundary conditions.

## INTRODUCTION

The boundary element method (BEM) has evolved within the last two decades as a powerful tool for solving a variety of problems in physics and engineering. The automatic reduction in the dimensionality of the problem is one of the major advantages BEM has enjoyed over the *domain* techniques such as finite element and finite difference methods.

One key difficulty in the use of BEM for serious real-life cases is the problem of ill-conditioning in the global matrix when a fine resolution is required in certain localities of the domain boundary. Examples include the formation of fractals in electrodeposition problems, cracks in fracture mechanics and fingering in soil moisture studies. Zoning has been suggested as a way of avoiding such problems (see Lafe *et al* [3]). However zoning increases the complexity and computational effort of the boundary solution process since artificial boundaries will then have to be introduced in the problem domain. The effect is an impairment of the user-friendliness in terms of the ease of data preparation normally associated with BEM codes.

Furthermore the incorporation of non-linear mixed boundary conditions (e.g. kinematic conditions in free-surface fluids problems or Tafel relationships in electrochemistry) is a rather difficult task in BEM. The solution process in such cases most often requires the inversion of the coefficient matrix several times. Such clumsy schemes destroy the traditional advantages of BEM.

In this paper we propose a simple but elegant solution scheme suitable for a variety of boundary integral problems. We call it the Iterative Boundary Element Method (I-BEM) in that the entire solution process is iterative even for linear equations with linear boundary conditions. The kernel of the method was first suggested by Cahan [1] and then implemented by Cahan *et al* [2]. The original scheme involved locating integration points near the boundary just inside of the problem domain and the use of finite differences as a predictor in the iterative process. The scheme is generalized in this paper to accommodate arbitrary choices of integration points on or off the boundary.



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A comprehensive description of the method is given here and we show how a relaxation factor $\lambda$ can be effectively used to accelerate the rate of convergence. We also examine the relative performances of I-BEM and BEM by solving a problem connected with the electrodeposition at an external corner. This problem is characterized by exponentially strong boundary conditions.

## GOVERNING DIFFERENTIAL EQUATION

For a domain $\Omega$ consisting of the boundary $\Gamma$ we look at a general class of problems governed by the differential equation:

$$\mathcal{L}'[\phi'(\mathbf{x},t)] = \mathcal{F}'(\mathbf{x}',t')\ \delta(\mathbf{x}',\mathbf{x}'') \tag{1}$$

where $\mathcal{L}'$ is some linear partial differential operator in both space $(\mathbf{x})$ and time $(t)$, $\phi'$ is the dependent variable (e.g. voltage, pressure, temperature, displacement, potential, stream function *etc*), $\delta$ is the Dirac delta function while $\mathcal{F}'$ represents the strengths of point *actions* or sources in $\Omega$.

By taking initial conditions as reference values we define $\phi = \int_0^\infty \phi' \exp(-st)dt$ where $s$ is the Laplace transform parameter and use these to transform equation (1) into:

$$\mathcal{L}[\phi(\mathbf{x},s)] = \mathcal{F}(\mathbf{x}',s)\ \delta(\mathbf{x}',\mathbf{x}'') \tag{2}$$

in which $\mathcal{L}$ is now a differential operator in space while $\mathcal{F}$ is the transform of $\mathcal{F}'$. In subsequent statements we drop the suffix $s$ without any loss of generality.

The conditions associated with the boundary $\Gamma$ can in general be written in the form:

$$f(\phi, \mathcal{D}[\phi], \mathbf{x}) = 0 \tag{3}$$

where $\mathcal{D}$ is another differential operator and $f$ is some prescribed function. On a Dirichlet boundary $f = f(\phi, \mathbf{x})$ while on a Neuman segment $f = f(\mathcal{D}[\phi], \mathbf{x})$ at most.

## INTEGRAL EQUATION

The first task in a BEM process is to convert the governing partial differential equation(1) into a suitable integral equation. This is achieved by multiplying the equation by a function $G$, integrating the ensuing expression over $\Omega$ and invoking the Green's identities or the Betti's reciprocal theorem. The result of such manipulations is the integral equation:

$$\int_\Omega \phi(\mathbf{x})\mathcal{L}^*[G(\mathbf{x},\mathbf{x}')]\ d\Omega = \int_\Gamma (\phi(\mathbf{x}')G^*(\mathbf{x},\mathbf{x}') - \phi^*(\mathbf{x}')G(\mathbf{x},\mathbf{x}')\ d\Gamma + \sum G(\mathbf{x},\mathbf{x}'')\mathcal{F}(\mathbf{x}'') \tag{4}$$

where $\mathcal{L}^*$ is the adjoint to operator $\mathcal{L}$ while $G^*$ and $\phi^*$ are derivative functions of $G$ and $\phi$ respectively. If we choose the function $G$ such that:

$$\mathcal{L}^*[G(\mathbf{x},\mathbf{x}')] = \delta(\mathbf{x},\mathbf{x}') \tag{5}$$

then equation(4) degenerates into:

$$\alpha\phi(\mathbf{x}) = \int_\Gamma (\phi(\mathbf{x}')G^*(\mathbf{x},\mathbf{x}') - \phi^*(\mathbf{x}')G(\mathbf{x},\mathbf{x}')\ d\Gamma + \sum G(\mathbf{x},\mathbf{x}'')\mathcal{F}(\mathbf{x}'') \tag{6}$$

where $\alpha$ is the Cauchy principal value of the integration of the Green's function singularity.

## COEFFICIENT MATRICES

To use the boundary element method the boundary $\Gamma$ is subdivided into a finite number of elements and suitable interpolation functions are chosen to represent the distribution of the dependent variables on the boundary. For function $\phi$ on $\Gamma$ we write:

$$\phi(\mathbf{x}) = \sum_i N_i(\mathbf{x})\phi_i \tag{7}$$

where $\phi_i$ are the values of $\phi$ at the discrete points on the boundary and $N_i$ are shape functions. A similar expression can be written for $\phi^*$. To perform boundary integrations we select a finite number of points to serve as integration origins such as $\mathbf{x}$ in equation(6). In most BEM implementations these points are located along the boundary segments and usually fall on the nodes formed at element intersections. In a few implementations (the so-called non-singular formulation) the integration points are selected outside $\Omega$. In I-BEM $\mathbf{x}$ can be placed on $\Gamma$, inside or outside of $\Omega$. The number of independent integration points selected is the same as the number, $M$, of all unknown $\phi$ or $\phi^*$ on the boundary.

When these integrations are performed equation(4) becomes:

$$\sum_{j=1}^{M} a_{ij}\phi_j = \sum_{j=1}^{M} b_{ij}\phi_j^* + c_i \quad i = 1, 2, \cdots, M \tag{8}$$

where

$$\begin{aligned} a_{ij} &= \int_{\Gamma_j} N_i^*(\mathbf{x}')G(\mathbf{x}, \mathbf{x}')\, d\Gamma \\ b_{ij} &= \int_{\Gamma_j} N_i(\mathbf{x}')G^*(\mathbf{x}, \mathbf{x}')\, d\Gamma \\ c_i &= \sum_k \mathcal{F}(\mathbf{x}_k)G(\mathbf{x}, \mathbf{x}_k) \end{aligned}$$

In a conventional BEM the boundary conditions will be introduced into the system of equations(8) and then assembled into the form:

$$\sum_{j=1}^{M} d_{ij}u_j = e_i \quad i = 1, 2, \cdots, M \tag{9}$$

where $u_j$ represents the unknown $\phi$ or $\phi^*$ at the $M$ nodes. Equation(9) is then inverted to obtain these unknown quantities. For problems with non-linear boundary conditions equation(9) becomes essentially a non-linear system of equations and the assembling process may even have to be repeated several times in order to take full advantage of available linear matrix inversion routines. The approach in I-BEM is different since the assembling symbolized by equation(9) is never carried out. Rather equation(8) is utilized directly.

## I-BEM

To solve for the unknown $\phi$ and $\phi^*$ at the nodes we start by guessing the values, $\phi_e$ and $\phi_e^*$ for these quantities. (Zeroes may be used for unfamiliar problems. The additional number of iterations required is usually small (2-3) when compared to the case when a more 'intelligent' initial guess is made.) For Dirichlet (exact $\phi_e$) and Neuman (exact $\phi_e^*$) type problems the known quantities can be used once and for all in equation(8) and the results absorbed into the coefficients $c_i$. For linear mixed boundary conditions one will normally eliminate either $\phi$ or $\phi^*$ for the other. In non-linear mixed conditions the iterative process readily accepts the incorporation of any root-finding routine in the solution process. When the guesses are used in the equation written for the $i$-th node as origin of integration [see equation(8)] the result is an error:

$$\varepsilon_i = \sum_{j=1}^{M} a_{i,j}\phi_{e_j} - \sum_{j=1}^{M} b_{i,j}\phi_{e_j}^* + c_i \tag{10}$$

Assuming the largest contributor to $\varepsilon_i$ comes from the $j = i$ terms the $j \neq i$ terms in equation(10) can be suppressed to obtain a suitable expression for updating the unknown(s) at the $i-$th node. The ensuing update equations are:

### Neuman Boundary

$$\phi_i = \phi_{e_i} - \lambda \frac{\varepsilon_i}{a_{ii}} \tag{11}$$

### Dirichlet Boundary

$$\phi_i^* = \phi_{e_i}^* + \lambda \frac{\varepsilon_i}{b_{ii}} \tag{12}$$

### Mixed Boundary

$$a_{ii}(\phi_i - \phi_{e_i}) - b_{ii}(\phi_i^* - \phi_{e_i}^*) = -\lambda\varepsilon_i \tag{13}$$

where $\lambda$ is an over-relaxation factor whose optimal choice is examined below. For a segment with a mixed boundary condition equation(13) is to be solved with the relevant prescribed condition as shown by equation(3).

The above process is repeated for all points until a suitable convergence criterion is satisfied.

## OPTIMAL $\lambda$-VALUES

An exact analysis of the optimal $\lambda$ is difficult to carry out. We present an approximate analysis which provides a sense of the best estimate for the over-relaxation factor.

We write error equation(10) for two iteration levels $k$ and $k+1$. By subtracting the ensuing expressions the result is:

$$\varepsilon_i^{k+1} - \varepsilon_i^k = \sum_{j=1}^{M} a_{i,j}(\phi_j^{k+1} - \phi_j^k) - \sum_{j=1}^{M} b_{i,j}(\phi_j^{*\,k+1} - \phi_j^{*\,k}) \tag{14}$$

Using equations (11) and (12) in (14) and rearranging we obtain:

$$\frac{\varepsilon_i^{k+1}}{\varepsilon_i^k} = 1 - \lambda \sum_{j=1}^{M} \left( \frac{\varepsilon_j^k}{\varepsilon_i^k} \right) \left[ \frac{a_{ij}}{a_{jj}} + \frac{b_{ij}}{b_{jj}} \right] \tag{15}$$

For convergence we must enforce:

$$\left| \frac{\varepsilon_i^{k+1}}{\varepsilon_i^k} \right| < 1$$

Assuming a uniformity in segment errors ($\varepsilon_j^k \approx \varepsilon_i^k$) equation (15) when combined with the above condition produces:

$$0 < \lambda < 2 / \sum_{j=1}^{M} \left[ \frac{a_{ij}}{a_{jj}} + \frac{b_{ij}}{b_{jj}} \right] \tag{16}$$

Since condition (16) would provide different limitations on the value of the $\lambda$s for different segment and our analysis assumed an *a priori* constant $\lambda$ for all segments the optimal choice has to be the value that satisfies the condition for all segments. That is in addition to being positive the optimal value has to be such that:

$$\lambda < \min 2 / \sum_{j=1}^{M} \left[ \frac{a_{ij}}{a_{jj}} + \frac{b_{ij}}{b_{jj}} \right] \quad i = 1, 2, \cdots, M \tag{17}$$

Numerical experiments have confirmed the validity of the above convergence criterion. The result shows the optimal $\lambda$ is dependent on geometry and the number of boundary elements.

## NUMERICAL RESULTS

The following numerical tests have been performed for a steady state boundary value problem governed by Laplace's equation (*i.e.* $\mathcal{L} = \nabla^2$ and $\mathcal{F} = 0$). The domain of study is as depicted in Fig(1).

The problem is connected with the electrodeposition process in which the condition on a portion the boundary is governed by the Butler-Volmer equation:

$$\frac{\partial \phi}{\partial n} = \kappa \left[ e^{\nu_1 \phi} - e^{-\nu_2 \phi} \right]$$

where $\kappa$, $\nu_1$ and $\nu_2$ are coefficients dependent on the material and kinetics of the reaction. In the special case when $|\phi| >> 1$ $\nu_2$ the Butler-Volmer equation degenerates to the so-called Tafel equation. In all the simulations linear shape functions have been used. Error plots for varying values of relaxation factors and number of of boundary elements are shown in Fig(2).

The iterative process was carried out over 3 passes. The maximum observed error is $4.9 \times 10^{-4}$. The minimum is $2.1 \times 10^{-5}$ for the 3 iterations. The optimal relaxation factor generally lies between 0.6 - 0.75. The higher value seems to be more appropriate for problems with relatively large number of elements. The convergence rate is reduced significantly when a small factor $< 0.2$ is used for many test runs that were made. The 0.75 upper limit is rigid for most problems as severe instabilities are common for relaxation factors just slightly higher than this value.

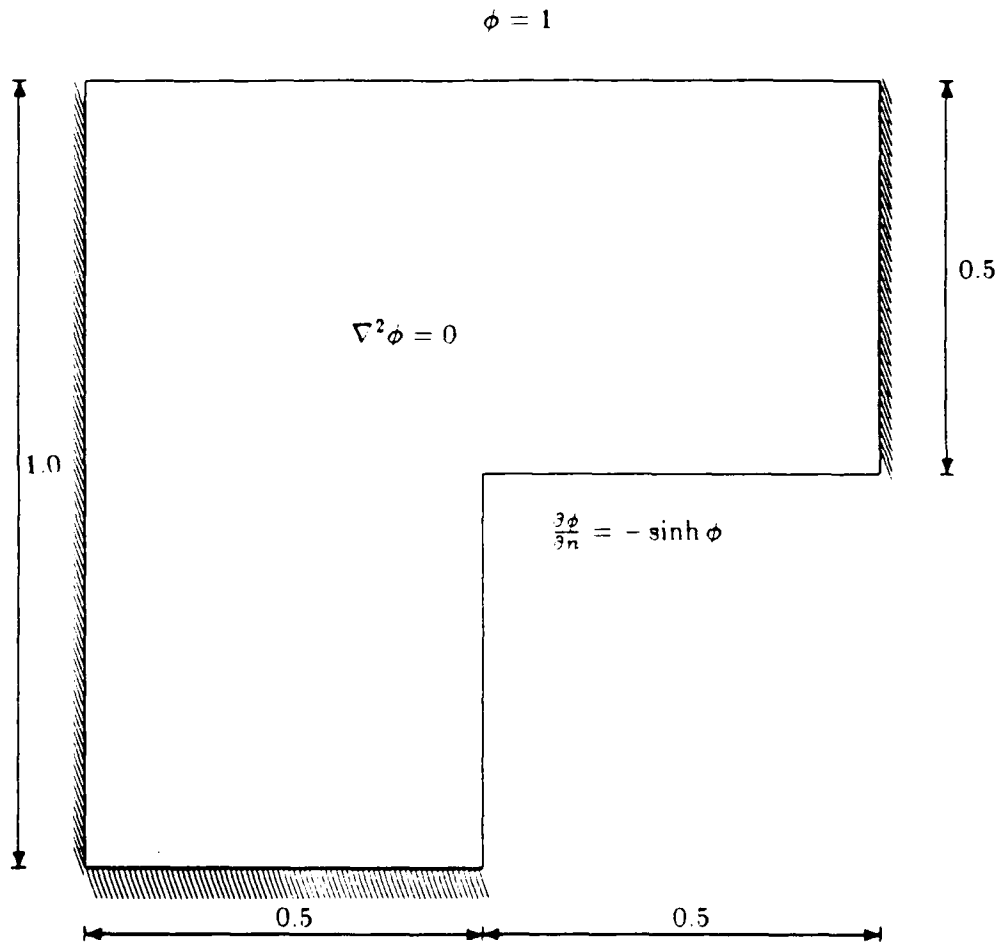


Figure 1: Electrodeposition at a corner

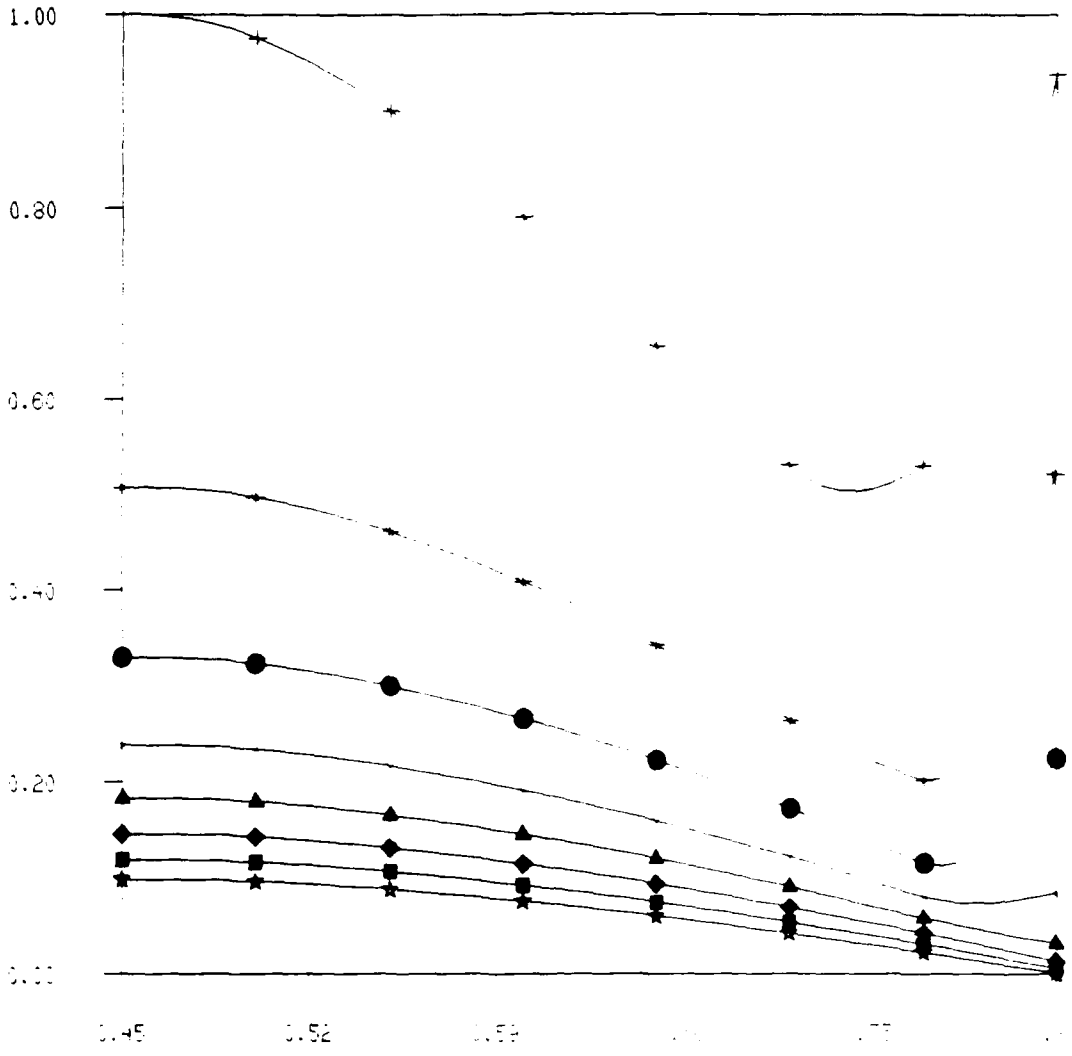


Figure 2: Error Plots for various $\lambda$ values and element size. Normalized error $= (\epsilon - \epsilon_{min})/(\epsilon_{max} - \epsilon_{min})$ ——— 10 elements segment; ——*—— 80 elements/segment

## I-BEM VERSUS BEM

In using BEM the presence of the Tafel segment means the the final global matrix is nonlinear. The solution process then even in that case still has to be iterative as mentioned earlier. The comparative central processing unit (cpu) time plots for both methods are shown in Fig(3). Both processes were limited to 3 iterations. While the typical error in I-BEM (with a $\lambda$ value of 0.7) was of the order $10^{-4}$ that of BEM was of order $10^{-2}$ at the end of the 3 iterations. The significant advantage enjoyed by I-BEM in terms of computational speed is quite evident from the two curves in Fig(3) especially as the number of elements is increased.

## CONCLUSIONS

The iterative boundary element method has been presented in this paper as a powerful tool for solving a wide class of boundary value problems. The advantages of the new scheme are much evident in large systems. A given problem with $M$ unknowns on the boundary typically requires $\mathcal{O}(M^3)$ arithmetic computations for the direct matrix inversion used in conventional BEM. In I-BEM the computational effort is $\mathcal{O}(I_{max}M^2)$ where $I_{max}$ is the total number of iterations required to reach convergence. Thus I-BEM enjoys a computational advantage of the order $M/I_{max}$ over BEM. In general the number of iterations necessary is orders of magnitude smaller than the number of unknowns. Lafe and Cheng [4] have reported the simulation of a stochastic flow problem in which the computational time using I-BEM for 1600 unknowns was 5% of the corresponding time required by BEM.

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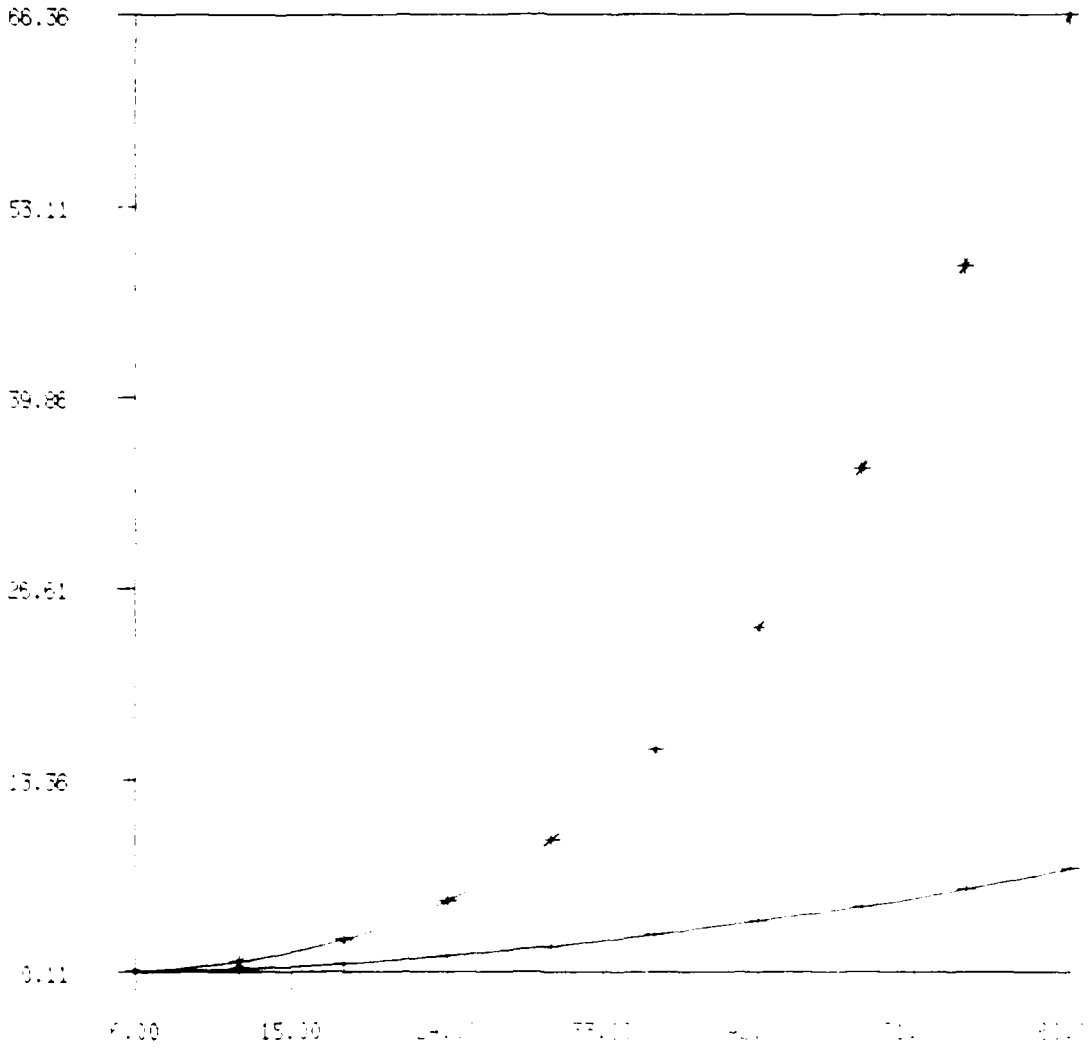


**Figure 3**: Comparative run-time plots for I-BEM and BEM. – – – * – – – → BEM; – – – + – – – — I-BEM